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НОВОСИБИРСК

The Hartree-Fock Calculation of Parity Violation in the Atomic Caesium, Induced by the Anapole Moment of the Nucleus

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ABSTRACT

The P-odd E1-transition amplitudes of $6s,F-7s,F'$ transitions in ^{133}Cs caused by the anapole moment of the nucleus are calculated by the relativistic Hartree—Fock method. The major part of correlation corrections is calculated using Brueckner orbitals. The correlation corrections and the contribution of states with $j \neq 1/2$ appeared to be small enough, so our result is close to the semiempirical result of Frantsuzov and Khriplovich.

1. INTRODUCTION

The P-odd interaction of atomic electrons with the nucleus contains a part depending of the spin of the nucleus. It causes the difference in P-odd properties of different hyperfine components of the same line. One of the possible types of such interaction is the interaction of electrons with the anapole moment of the nucleus [1, 2]. The major contribution to the anapole moment of the heavy nuclei is due to the P-odd nuclear forces [1, 2]. The weak interaction between the electron vector and nucleon axial neutral currents has the same radial and angular dependence, so these interactions are indiscernable in atomic experiments. The total interaction is characterized by the constant $\varkappa$:

$$W_a = \frac{G\left(I+\frac{1}{2}\right)(-1)^{I+l+\frac{1}{2}}}{\sqrt{2}\ I(I+1)} \varkappa\, \rho_n(\vec{r})\, \vec{I}\vec{\alpha}\,, \qquad (1)$$

where G is the Fermi constant, $\vec{I}$—the spin of the nucleus, l—the orbital moment of the external nucleon, ρ_n—the nucleon density, normalized to unit, $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$—the Dirac matrix. For heavy nuclei, the $\varkappa$ constant is about 0.2—0.4 [2].

The P-odd E1-transition amplitudes caused by the nucleus anapole moment have already been calculated for thallium, lead, bismuth [3] and caesium [3, 4] atoms. In these calculations the E1-amplitudes were obtianed in the second order of the perturbation

theory:

$$(\mathrm{E1})_{\gamma\gamma'} = -\sum_{\gamma''}\left(\frac{\langle\gamma|W_a|\gamma''\rangle\langle\gamma''|\mathrm{E1}|\gamma'\rangle}{\varepsilon_{\gamma''}-\varepsilon_{\gamma}} + \frac{\langle\gamma|\mathrm{E1}|\gamma''\rangle\langle\gamma''|W_a|\gamma'\rangle}{\varepsilon_{\gamma'}-\varepsilon_{\gamma'}}\right). \qquad (2)$$

The matrix elements of P-odd interaction (1) were calculated in quasi-classical approximation (for heavy atoms the electron wave functions at the small radii may be normalized by joining the quasi-classical wave functions (see, for example, [5])). The difference of the exact electron wave functions at the nucleus from the «quasi-classical» ones was also taken into account [4]. For this purpose the results of «quasi-classical» calculation of hyperfine constants were compared with the experiment. The experimental values of radial integrals and energies of allowed E1-transitions were used.

In the sum (2) only the intermediate states $p_{1/2}$ (for $s_{1/2}-s_{1/2}$ P-odd transitions) and $s_{1/2}$ (for $p_{1/2}-p_{1/2}$ and $p_{1/2}-p_{3/2}$ ones) were considered because the interaction (1) is localized at the nucleus and only the $s_{1/2}$ and $p_{1/2}$ electron wave functions are not small there. Such limited sum is not sufficient when the polarization, caused by the P-odd wave function perturbations, is taken into account. Firstly, the perturbation of the Coulomb potential causes the P-odd perturbations of all the wave functions, rather than $s_{1/2}$ and $p_{1/2}$ ones. Secondly, the interaction (1) is vector one and can cause the transitions with changes of angular momentum by unit. So, all the P-odd matrix elements with $\Delta j = 0, \pm 1$ must be taken into account in the sum (2).

In the present work the P-odd E1-amplitudes of $6s,F-7s,F'$ transitions in ^{133}Cs atom due to the anapole moment of the nucleus are calculated by the relativistic Hartree—Fock method. The contributions of polarization and $\Delta j \neq 0$ transitions are determined. The major part of correlation corrections is calculated using Brueckner orbitals.

2. CALCULATION

The calculation is very similiar to that for the spin-independent weak P-odd electron-nucleon interaction [6]. This made it possible to use a set of computer programs, developed earlier [6]. The main feature of the present calculation is connected with the vector character of interaction (1).

The P-odd wave function perturbations $\delta\varphi$ caused by the electron part of interaction (1) $W_e = \rho_n(\vec{r}\,)\vec{\alpha}$ were calculated with taking into account the exchange polarization δV_W (the direct polarization in first order on $\delta\varphi$ is equal to zero). Then the wave function perturbations caused by the external alternating electric field were calculated also with the account for the polarization (the time-dependent Hartree—Fock calculation, TDHF [6], with the frequency of the external field $\omega = \varepsilon_{7s} - \varepsilon_{6s}$). These perturbations were necessary to determine the polarization δV_E which describes the shielding of external electric field inside the atom. Then the resulting P-odd E1-transition amplitudes were calculated:

$$(\mathrm{E1})_{F'F} = \langle\delta\varphi_{7s,F'}|\mathrm{E1}+\delta V_E|6s,F\rangle + \langle 7s,F'|\mathrm{E1}+\delta V_E|\delta\varphi_{6s,F}\rangle.$$

The diagrams of the zero and first order on Coulomb interaction composing this result are shown at Figs. 1,*a*—1,*d*. Our calculation differs from the random phase approximation with exchange

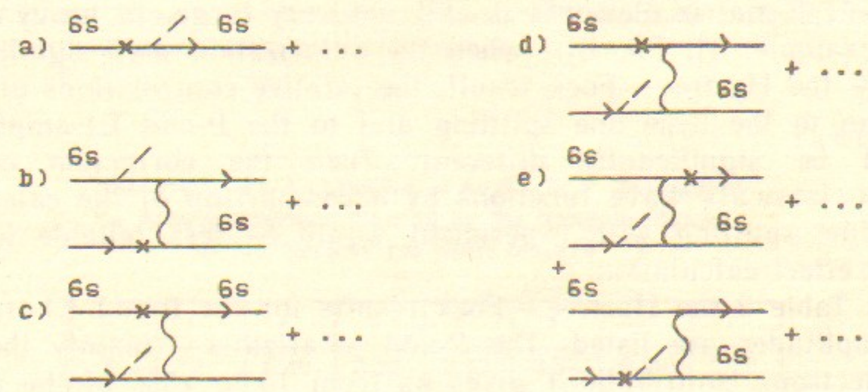

Fig. 1. The diagrams of zero and first order on Coulomb interaction, which take part in the RPAE approximation. Diagrams 1,*e* were not taken into account in our calculations.

}—the Coulomb electron-electron interaction; ×—the P-odd electron-nucleus interaction; /—the interaction of electron with external field.

(RPAE) because the 1,*e* diagram contribution was not calculated. In the case of spin-independent P-odd interaction in atomic caesium [6] the 1,*e* diagrams contain 0.2% of the total result.

The part of correlation corrections in the second order on Coulomb interaction which corresponds to the renormalization of the external electron wave functions was calculated using the Brueckner orbital method. This part of correlations must dominate [7]: the

rest part of corrections should be $\varepsilon_{ext}/\varepsilon_{in}$ times smaller. Here ε_{ext}, ε_{in} are the typical energies of external and inner shell electrons correspondingly. For caesium this parameter is $\varepsilon_{6s}/\varepsilon_{5p} \simeq 0.15$.

3. RESULTS

The calculation of P-odd matrix elements $\langle\gamma'|\delta\varphi_\gamma\rangle = -\langle\gamma'|W_e+\delta V_W|\gamma\rangle/\Delta\varepsilon_{\gamma'\gamma}$ (Table 1) confirms the previous speculations about the influence of the P-odd polarization. It causes the 30% increase of the $s_{1/2}-p_{1/2}$ matrix elements and the strong increase of the rest matrix elements. The matrix elements were calculated also in the approximation when only the $s_{1/2}$ and $p_{1/2}$ electrons make the contributions to the polarization. The matrix elements with Brueckner orbitals are close to that calculated earlier with the corrected values of electron wave functions at the nucleus [4]. This coincidence happens because the contributions of polarization to the $j=j'=1/2$ matrix elements is still not very large. In heavy atoms (for example, Tl, Pb, Bi), when the polarization may significantly change the Hartree—Fock result, the relative contributions of polarization to the hyperfine splitting and to the P-odd E1-amplitudes would be significantly different. Then the correction of the «quasi-classical» wave functions by a comparison of the calculated hyperfine splitting with experiment would be less reliable for the P-odd effect calculation.

In Table 2 the Hartree—Fock results for the P-odd E1-transition amplitudes are listed. The P-odd polarization (mainly the $s_{1/2}$, $p_{1/2}$-electrons contribution) gives us from 15 to 25% of the result. The correlation corrections are about 4%. Approximately the same contribution (about 5%) is due to the states with $j\neq 1/2$ not taken into account earlier [3, 4], so the exact coincidence of our E1-amplitudes for $F=F'$ with the result [4] is to some extent accidental one.

4. CONCLUSION

In the Hartree—Fock calculation of P-odd E1-transition amplitudes in the atomic caesium caused by the anapole moment of the nucleus the contribution of the P-odd polarization is significant. The contributions of states with $j\neq 1/2$, transitions with $\Delta j\neq 0$ and of correlation corrections are observable but not large. Hence, the

Table 1.

The P-Odd Matrix Elemeq ts $\langle\gamma'|\delta\varphi_\gamma\rangle = -\langle\gamma'|W_e+\delta V_W|\gamma\rangle/\Delta\varepsilon_{\gamma'\gamma}$ in Caesium Atom (Atomic Units)

γ	$6s_{1/2}$				$7s_{1/2}$			
γ'	$6p_{1/2}$	$7p_{1/2}$	$6p_{3/2}$	$7p_{3/2}$	$6p_{1/2}$	$7p_{1/2}$	$6p_{3/2}$	$7p_{3/2}$
a	29.6	8.66	−0.022	−0.007	−21.2	29.5	0.018	−0.023
b	38.4	11.2	0.45	0.12	−27.6	37.9	−0.44	0.51
c	42.6	12.2			−32.2	39.0		
d	38.1	11.1	1.05	0.30	−27.4	37.8	−0.93	1.07
e	42.2	12.4			−32.0	39.0		
f	45.1	13.0			−33.4	42.7		

a—without polarization; b—with polarization, caused by $s_{1/2}$, $p_{1/2}$ wave function perturbation; c—with $s_{1/2}$, $p_{1/2}$ polarization and Brueckner orbitals; d—with polarization of all the states; e—with total polarization and Brueckner orbitals (the complete result); f—the quasi-classical calculation [4].

Table 2.

The P-Odd E1-Amplitudes of $6s,F-7s,F'$ Transitions in Atomic Caesium, Caused by the Anapole Moment of the Nucleus (in Units $ieа_B\times10^{-12}$)

F	F'	a	b	c*	d	e	f
3	3	0.49	0.60	0.62 (2)	0.57	0.59 (2)	0.59 (3)
3	4	1.21	1.62	1.68 (3)	1.64	1.70 (2)	1.73 (4)
4	3	1.40	1.85	1.92 (4)	1.86	1.92 (2)	1.96 (4)
4	4	0.56	0.68	0.70 (2)	0.65	0.67 (2)	0.68 (4)

a—f — the same, as in Table 1; *—in parentheses—the numerical uncertainties.

result does not significantly differ from the semiempirical one [4]. The polarisation and correlation contributions must be more significant for heavy atoms (Tl, Pb, Bi). For these atoms the semiempirical methods become less reliable and the Hartree—Fock method with calculation of correlations is necessary.

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